

Non-Invasive Vapor Liquid Equilibrium Measurements

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An understanding of the vapor-liquid equilibrium (VLE) of mixtures is imperative for optimizing chemical separations, which can account for 50-80% of industrial production costs. Some of the most important mixtures that are of concern in industry can be classified as reactive, corrosive and toxic (RCT). There is very little VLE information available on these mixtures primarily because of difficulties in chemically analyzing these systems, and because of uncertainties caused by molecular associations. A non-invasive Fourier transform infrared (FTIR) analytical method has been developed to simultaneously measure the liquid and vapor phases of RCT mixtures without sample withdrawal, allowing reliable VLE data to be obtained without perturbing the equilibrium. The experimental apparatus consists of a high-pressure, high-temperature equilibrium vessel that accommodates an infrared transmission probe to monitor the vapor phase and an attenuated total reflectance (ATR) probe to monitor the liquid phase. The vessel also contains a gas-liquid entraining rotor to ensure efficient mixing of the phases and rapid phase equilibration. With infrared spectroscopy, intermolecular associations are immediately apparent through frequency shifts, enabling comprehensive interpretation of results. In addition to providing crucial VLE, this approach will allow intermolecular associations to be correlated with theoretical models, providing industry with new predictive capabilities for numerous complex mixtures. The operation and applicability of the apparatus will be illustrated with several isotherms of the CO₂-n-butane VLE system, and mixture of a refrigerant and a lubricant.